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Effective medium approach for planar QD structures

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Abstract. The effective boundary condition (EBC) method is extended to nano-scale planar mesoscopic systems. The EBCs appear as a result of the 2D-homogenization procedure and have the form of two-side anisotropic impedance boundary conditions stated on the structure surface. The EBC method supplemented with well-developed mathematical techniques of classical electrodynamics creates unified basis for solution of boundary-value problems in electrodynamics of quantum dots.

1. Introduction

The key peculiarities of quantum dot (QD) heterostructures [1] are related to spatial confinement of the charge carrier motion and intrinsic spatial inhomogeneity. Since the inhomogeneity scale is much less than the optical wavelength, QDs can be treated as *electrically small* objects and electromagnetic response of such structures can be evaluated by means of effective medium theory. Effective medium approach as applied to 3D arrays of QDs has been developed in Refs. [2, 3]. In this paper we present a general method which allows us to evaluate electromagnetic response of planar arrays of QDs and to establish correlation between properties of such systems and homogeneous 2D structures like quantum wells (QWs). This method, the effective boundary condition (EBC) method, has been originally developed for microwaves and antenna theory (see, e.g., [4]) and is modification of the effective medium theory as applied to 2D-confined structures. Its basic idea is that a smooth homogeneous surface is considered instead of the initial structure, and appropriate EBCs for the electromagnetic field are stated for this surface. These conditions are chosen in such a way that the spatial structure of the field due to an effective current, and the field of the real current in the initial structure turn out to be identical at some distance away from the surface. Material characteristics of the structure and its geometrical parameters are included in coefficients of the EBCs.

2. EBCs for planar nanostructures

Under the derivation of EBCs, the kernel problem is the diffraction of electromagnetic field by an infinite planar quadratic lattice constituted by identical QDs imbedded in a host medium whose permittivity ε_h is assumed to be real-valued and dispersionless. In the strong confinement regime, when the exciton Bohr radius exceeds significantly the QD linear extension ($a_B \gg R$), the Lorentz dispersion law $\varepsilon(\omega) = \varepsilon_h + g_0/(\omega - \omega_0 + i/\tau)$ can be used as model of dispersion in a single QD in the vicinity of the exciton resonance [5]; here ω_0 is the frequency of the transition, τ is the effective exciton dephasing time in the QD, $g_0 = -4\pi\mu^2 W/\hbar V$ where μ and V are the QD dipole moment and volume, W is the level population difference ($W < 0$ in an inverted medium).

In the dipole approximation, electromagnetic field scattered from an isolated QD can be expressed in terms of Hertz potentials by

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_0(\mathbf{r}) + \sum_{l,m=-\infty}^{\infty} \left[\nabla \nabla \cdot \mathbf{\Pi}_{lm}^e(\mathbf{r}) + k_1^2 \mathbf{\Pi}_{lm}^e(\mathbf{r}) \right]. \quad (1)$$

Corresponding equation for the magnetic component is also presented. Here $k = \omega/c$, $k_1 = k\sqrt{\varepsilon_h}$, $\mathbf{E}_0(\mathbf{r})$ stands for the incident field; an $\exp(-i\omega t)$ time-dependence is supposed. Further the incident field is assumed to be \mathbf{e}_x -polarized plane wave propagating at angle θ with respect to the z axis. Hertz potentials are given by

$$\mathbf{\Pi}_{lm}^e(\mathbf{r}) = \left[\mathbf{e}_x \alpha_{xx} \mathcal{E}_x(\mathbf{R}_{lm}) + \mathbf{e}_z \alpha_{zz} \mathcal{E}_x(\mathbf{R}_{lm}) \right] \frac{\exp(ik_1 |\mathbf{r} - \mathbf{R}_{lm}|)}{|\mathbf{r} - \mathbf{R}_{lm}|}, \quad (2)$$

where $\mathbf{R}_{lm} = \{ld, md, 0\}$ is the radius-vector of a lattice site, d is the lattice period, α_{ii} are the components of the QD polarizability tensor $\hat{\alpha}$, and $\mathcal{E}(\mathbf{r})$ is the electric field inside QD. This field is related to the Hertz potentials by the equation analogous to Eqs. (1) in the limit $\mathbf{r} \rightarrow 0$ with the term $l = m = 0$ excluded. For QDs with planar configuration in the xOy plane, e.g., discs, islands, flattened pyramids, etc., the QD polarizability in the z direction α_{zz} can be neglected.

The next step is the 2D-averaging of the electromagnetic field in the $z = 0$ plane. Such a procedure implies replacement of the discrete 2D elementary scatterer by a homogeneous $d \times d$ surface element; mathematically this procedure reduces summation in equations for inner and outer fields to integration. Then, one should find discontinuities of the mean field tangential components at $z = 0$ taking into account that the mean field has $\exp(ik_1 x \sin \theta)$ dependence on the x co-ordinate. Then, after some manipulations, we come to the covariant notation of the EBCs:

$$\begin{aligned} \mathbf{n} \times \mathbf{n} \times (\mathbf{H}^I - \mathbf{H}^{II}) &= -\frac{2\pi}{c} \hat{\sigma} \mathbf{n} \times (\mathbf{E}^I + \mathbf{E}^{II}), \\ \mathbf{n} \times (\mathbf{E}^I - \mathbf{E}^{II}) &= -\xi \mathbf{n} \times \nabla [\mathbf{n} \cdot (\mathbf{E}^I + \mathbf{E}^{II})] \end{aligned} \quad (3)$$

where

$$\hat{\sigma} = \begin{pmatrix} \hat{\sigma}_{\parallel} & 0 \\ 0 & 0 \end{pmatrix}, \quad \hat{\sigma}_{\parallel} = i \frac{\omega \varepsilon_h}{d^2} \hat{\alpha}_{\parallel} \left(\hat{\mathbf{I}}_{\parallel} + \frac{\delta_x}{d^2} \hat{\alpha}_{\parallel} \right)^{-1}, \quad \xi = \frac{2\pi \alpha_{zz}}{d^2 + \delta_z \alpha_{zz}}. \quad (4)$$

Here, $\hat{\mathbf{I}}_{\parallel}$ is the 2×2 unit tensor and $\hat{\alpha}_{\parallel}$ is the surface polarizability tensor with components α_{ij} ($i, j = x, y$); $\delta_x \approx -8/\sqrt{2}d$, $\delta_z \approx 2\pi\sqrt{\pi}/d$.

The equations (3) and (4) constitute the complete system of EBCs for electromagnetic field in planar QD structures. The technique of macroscopic averaging used under their derivation is similar to one which introduces the constitutive parameters for bulk media, but differs in that the averaging occurs in boundary conditions rather than in field equations. Thus, in electrodynamics of low-dimensional structures the EBCs play the same role as constitutive relations in electrodynamics of bulk media. The EBCs keep validity for arbitrary configuration of elementary cell and for planar layers with random distribution of QDs. The difference will manifest itself in the modified coefficients δ_i . Since EBCs (3) are local and the coefficients $\hat{\sigma}_{\parallel}$, ξ do not depend on the angle of incidence θ , they are applicable at arbitrary excitation in spite of that they have been obtained originally for plane waves. Moreover, the EBCs (3) are analogous to corresponding EBCs for QWs (see,

e.g., [3]) if spatial dispersion in the latter can be neglected. Thus, a planar layer comprising a 2D array of QDs can be treated as an effective QW. As a result, well-developed formalism of investigation of QWs can be extended to QD arrays by introducing of effective integral parameters of the array defined by Eqs. (4).

3. The role of nonlocality

In the weak confinement regime, the QD electromagnetic response becomes nonlocal and the medium polarization takes the form of the integral operator [7]:

$$\mathbf{P}(\mathbf{r}) = A\Phi(\mathbf{r}) \int_V \Phi(\mathbf{r}')\mathbf{E}(\mathbf{r}') d^3\mathbf{r}', \quad (5)$$

where $A \sim 1/(\omega - \omega_0 + i/\tau)$, $\Phi(\mathbf{r})$ is the envelope function of the exciton ground state. Eq. (5) defines very special type of nonlocality: the integral operator has degenerated kernel. This property makes possible analytical consideration of the nonlocality problem: integral differential equations describing electromagnetic field in QD turn out to be equivalent to the integral Fredholm equations with degenerated kernels. As a result, we obtain the polarizability tensor of an isolated QD as $\hat{\alpha} = AN^2(\hat{\mathbf{I}} - 4\pi A\hat{\Upsilon})^{-1}$, where the 3D-tensor $\hat{\Upsilon}$ is given by

$$\Upsilon_{\alpha\beta} = \frac{1}{4\pi} \int_V \int_V \Phi(\mathbf{r})\Phi(\mathbf{r}') \frac{\partial^2}{\partial x_\alpha \partial x_\beta} \frac{1}{|\mathbf{r} - \mathbf{r}'|} d^3\mathbf{r} d^3\mathbf{r}' \quad x_\alpha, x_\beta = x, y, z. \quad (6)$$

Thus, we have shown that the nonlocality changes values of the polarizability tensor components but does not change the general representation of the scattering operators as compared to the strong confinement regime. This allows us to conclude that the above introduced EBCs remain valid in the weak confinement regime as well. Note that the above result admits extension of the Maxwell Garnett approach to 3D composites constituted by QDs in weak confinement regime.

4. Radiative decay rate in planar array of QDs

Let us apply the EBC method for the investigation of exciton radiative time in 2D-array of QDs which are assumed to be spherical inclusions of the radius R . The problem of the radiative linewidth evaluation in QWs is solved by finding of the frequency poles of the reflection coefficients [8]. Real parts of these poles determine resonant frequencies while imaginary parts give the homogeneous linewidths. It can easily be shown that EBCs (3) with $\hat{\sigma}_\parallel = ick\eta\hat{\mathbf{I}}_\parallel/4\pi$, $\xi = -\eta/2\varepsilon(\omega)$ and $\eta = L_{\text{QW}}[\varepsilon(\omega) - \varepsilon_h]$ describe a QW with L_{QW} as its thickness. Thus, the reflection coefficient for planar array of spherical QDs are given by a corresponding equation for QW after substitutions $L_{\text{QW}} \rightarrow 2R$, $g_0^{\text{QW}} \rightarrow g_0^{\text{eff}} \approx (2\pi R^2/3d^2)g_0$ and $\omega_0 \rightarrow \tilde{\omega}_0 = \omega_0 - g_0/3\varepsilon_h$. Then, using results of Ref. [3] and above denoted substitutions, we obtain the expressions $\Gamma_p = \Gamma_0/\cos\theta$, $\Gamma_s = \Gamma_0 \cos\theta$, for TE and TM polaritons, correspondingly; here

$$\Gamma_0 \approx -\frac{2\pi}{3\sqrt{\varepsilon_h}} \frac{R^2}{d^2} \frac{\tilde{\omega}_0}{c} R g_0, \quad (7)$$

Comparison of Γ_0 with the radiative decay rate of a single spherical QD γ gives us $\Gamma_0/\gamma = B \approx 3\pi/(k_1 d)^2$. In dense arrays of QDs $B \gg 1$ signaling significant enhancement of

the decay rate Analogous superradiance factor with the Bohr radius a_B instead of d was introduced also for QWs [2]. One can interpret the coefficient B in close analogy with Ref. [2]: it results from the coherent excitation of QDs located at distance d from each other.

5. Conclusion

EBCs given by Eqs. (3) state mathematical equivalence of optical properties of a 2D periodical layer of QDs and an isolated QW. It should be stressed that the mechanisms of transport processes and oscillator strengths in each case are essentially different. Nevertheless, the equivalence makes it possible to extend to QD-based planar structures with more complicated configurations (finite-sized QD layer, QD layer in microcavity, several QD layers, etc.) the well-developed mathematical formalism of investigation of QWs. Namely this equivalence provides promising potentiality of the derived EBCs for particular electrodynamical problems in QD-based structures. In particular, threshold current for QD-based lasers can be evaluated by analogy with solution of corresponding problem for the QW lasers; the EBC method allows us to analyze electromagnetic response of a QD layer (or a multilayer structure) placed in microcavity: this is very important for the design of QD-based semiconductor lasers [1].

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